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## Fluctuation-induced forces in periodic slabs: Breakdown of $\epsilon$ expansion at the bulk critical point and revised field theory

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**Abstract.** – Systems described by n-component  $\phi^4$  models in a  $\infty^{d-1} \times L$  slab geometry of finite thickness L are considered at and above their bulk critical temperature  $T_{c,\infty}$ . The renormalization-group improved perturbation theory commonly employed to investigate the fluctuation-induced forces ("thermodynamic Casimir effect") in  $d=4-\epsilon$  bulk dimensions is re-examined. It is found to be ill-defined beyond two-loop order because of infrared singularities when the boundary conditions are such that the free propagator in slab geometry involves a zero-energy mode at bulk criticality. This applies to periodic boundary conditions and the special-special ones corresponding to the critical enhancement of the surface interactions on both confining plates. The field theory is reorganized such that a small- $\epsilon$  expansion results which remains well behaved down to  $T_{c,\infty}$ . The leading contributions to the critical Casimir amplitudes  $\Delta_{\rm per}$  and  $\Delta_{\rm sp,sp}$  beyond two-loop order are  $\sim (u^*)^{(3-\epsilon)/2}$ , where  $u^* = O(\epsilon)$  is the value of the renormalized  $\phi^4$  coupling at the infrared-stable fixed point. Besides integer powers of  $\epsilon$ , the small- $\epsilon$  expansions of these amplitudes involve fractional powers  $\epsilon^{k/2}$ , with  $k \geq 3$ , and powers of  $\ln \epsilon$ . Explicit results to order  $\epsilon^{3/2}$  are presented for  $\Delta_{\rm per}$  and  $\Delta_{\rm sp,sp}$ , which are used to estimate their values at d=3.

Fluctuations associated with long wave-length, low-energy excitations play a crucial role in determining the physical properties of many macroscopic systems. When such fluctuations are confined by boundaries, walls, or size restrictions along one or several axes, important effective forces may result. In those cases where the continuous mode spectrum that emerges as the system becomes macroscopic in all directions is not separated from zero energy by a gap, these fluctuation-induced forces are long-ranged, decaying algebraically as a function of the relevant confinement length L (separation of walls, thickness of the system, etc).

A prominent example of such forces are the Casimir forces [1] induced by vacuum fluctuations of the electromagnetic field between two metallic bodies a distance L apart [2–4]. Analogous long-range effective forces occur in condensed matter systems as the result of either (i) thermal fluctuations at continuous phase transitions or else (ii) Goldstone modes and similar "massless" excitations [5–12]. In particular the former ones, frequently called "critical Casimir forces," have attracted considerable theoretical and experimental attention recently. Beginning with the seminal paper by Fisher and de Gennes [5], they have been studied theoretically for more than a decade using renormalization group (RG) [6–10] and conformal field theory methods [13], exact solutions of models [12], as well as Monte

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2 EUROPHYSICS LETTERS

Carlo (MC) simulations [14–16]. Though their detailed experimental investigation just began, recent experiments [17–21] have provided clear evidence of their occurrence.

The goal of the present work is to reexamine the existence of the  $\epsilon=4-d$  expansion for critical Casimir forces. Considering n-component  $\phi^4$  models in  $\infty^{d-1} \times L$  slab geometries, subject to different kinds of large-scale boundary conditions (BC), we shall show that for some of these BC, the  $\epsilon$  expansion breaks down at the bulk critical temperature  $T_{c,\infty}$  beyond two-loop order because of infrared singularities. This breakdown occurs quite generally whenever the two-point correlation function in Landau theory has a zero mode at bulk criticality, as it does for periodic BC and for those corresponding to critical enhancements of the short-range surface interaction at both walls [22, 23].

As we shall show, the infrared problems one has in these cases require a special treatment of the zero mode. This leads to a modified RG-improved perturbation expansion, which is well-defined at and above  $T_{c,\infty}$ , but yields contributions to the critical Casimir force of the form  $(u^*)^{(3-\epsilon)/2}$  beyond two-loop order, where  $u^* = O(\epsilon)$  is the value of the renormalized  $\phi^4$  coupling constant at the infrared-stable fixed point in  $d = 4 - \epsilon$  bulk dimensions. Thus, contrary to common belief, this quantity does not generally have an expansion in integer powers of  $\epsilon$ ; the present theory requires fundamental revision.

That zero modes may play an important role and require special treatment has been observed before in studies of finite-size effects in systems that are finite in all, or in all but one, directions [24]. Such systems (with short-range interactions) differ from the ones in slab geometry considered here in that they do not have a sharp phase transition at T > 0, except in the bulk limit.

To put things in perspective, consider a system in a  $\infty^{d-1} \times L$  slab geometry whose bulk  $(L \to \infty)$  critical behavior is representative of the universality class of the d-dimensional n-component  $\phi^4$  model with short-range interactions. Its reduced free energy per unit cross-sectional area  $A \to \infty$  can be decomposed as

$$f_L \equiv \lim_{A \to \infty} \frac{F}{Ak_B T_{c,\infty}} = L f_{bk} + f_{s,a} + f_{s,b} + f_{a,b}^{res}(L) , \qquad (1)$$

where  $f_{\rm bk}$  is the reduced bulk free energy per volume, while  $f_{s,a} + f_{s,b}$  is the surface excess free energy that results as the separation L of the two confining plates is increased to infinity. According to the theory of finite-size scaling, the residual free energy should take the scaling form

$$f_{a,b}^{\text{res}}(L) \approx L^{-(d-1)} \Theta_{a,b}(L/\xi_{\infty})$$
 (2)

on sufficiently large length scales, where  $\xi_{\infty}$  is the bulk correlation length. Here  $\Theta_{a,b}$  is a universal scaling function, which depends on the bulk universality class, the geometry of the system, and gross properties of the confining planes, such as large-scale boundary conditions (BC) associated with RG fixed points of the corresponding boundary field theory, but is independent of microscopic details. Its value at bulk criticality,  $\Delta_{a,b} \equiv \Theta_{a,b}(0)$ , is a universal number, the so-called Casimir amplitude.

The so far most comprehensive and detailed theoretical investigation of critical Casimir forces is that of Krech and Dietrich (KD) [8,9] who considered n-component  $\phi^4$  models in a  $\infty^{d-1} \times L$  slab geometry whose Hamiltonian is given by

$$\mathcal{H}[\phi] = \int_0^L dz \int_{\mathbb{R}^{d-1}} d^{d-1}r \left[ \frac{1}{2} (\nabla \phi)^2 + \frac{\mathring{\tau}}{2} \phi^2 + \frac{\mathring{u}}{4!} \phi^4 \right]$$
(3)

together with BC. KD considered periodic (per) and antiperiodic (ap) BC, as well as (a,b)=(D,D),  $(D,\mathrm{sp})$ , and  $(\mathrm{sp},\mathrm{sp})$ . The notations D and  $\mathrm{sp}$  indicate Dirichlet and special BC on the boundary planes  $\mathfrak{B}_1$  at z=0 and  $\mathfrak{B}_2$  at z=L. The Dirichlet BC corresponds to the infrared-stable fixed point describing the surface critical behavior at the ordinary transition of semi-infinite systems. By special, the large-scale BC on a plate is meant that applies when the surface interactions on it are critically enhanced and no symmetry breaking surface terms are present there; they pertain to the fixed

point associated with the so-called special transition [22]. All combinations (a,b) of such BC with a,b=D, sp can be implemented by adding surface terms  $\sum_{j=1}^2 \int_{\mathfrak{B}_j} \mathring{c}_j \, \phi^2/2$  to the Hamiltonian (3) with  $\mathring{c}_j = \infty$  or  $\mathring{c}_j = \mathring{c}_{\mathrm{sp}}$  (critical enhancement [25]), depending on whether a,b=D, sp.

Performing two-loop calculations of the excess free energies, Casimir forces, and their scaling functions for the BC  $\wp=\operatorname{per}$ , ap, (D,D),  $(D,\operatorname{sp})$ , and  $(\operatorname{sp},\operatorname{sp})$ , and restricting themselves to temperatures  $T\geq T_{c,\infty}$ , KD obtained expansions to first order in  $\epsilon$  of the Casimir amplitudes  $\Delta_{\wp}$  and the scaling functions  $\Theta_{\wp}(y)$ .

The restriction  $T \geq T_{c,\infty}$  had not only technical reasons. As T is lowered beneath  $T_{c,\infty}$ , a crossover to the critical behavior of an effectively d-1 dimensional system is expected to occur at a temperature  $T_{c,L} < T_{c,\infty}$ . The  $\epsilon$  expansion is unable to deal with the d-1 dimensional infrared singularities at  $T_{c,L}$  since the appropriate small dimensional parameter would be  $\epsilon_5 \equiv 5-d$ . KD were aware of this problem. They verified that their  $O(\epsilon)$  results for the boundary conditions  $\wp =$  ap, (D,D), and  $(D,\operatorname{sp})$  were consistent with the asymptotic behavior of the scaling functions  $\Theta_\wp(y)$  for  $y\to 0\pm$  one can infer from the requirement that  $f_L$  be analytic at  $T_{c,\infty}$  when  $L<\infty$ . They also noted that one could not expect their results for  $\Theta_{\operatorname{per}}$  and  $\Theta_{\operatorname{sp,sp}}$  to exhibit such a small-y behavior because the corresponding free propagators with periodic and Neumann boundary conditions could not be analytically continued to negative values of  $\tau\sim (T-T_{c,\infty})/T_{c,\infty}$ , unlike those for the other boundary conditions. In order to assess the predictive power of their  $O(\epsilon)$  results for  $\Theta_\wp$ , KD (and others [12, 26]) nevertheless extrapolated these functions for all five types of boundary conditions to d=3 by setting  $\epsilon=1$ .

To see that the  $\epsilon$  expansion breaks down at  $T = T_{c,\infty}$  for  $\wp = \text{per}$  and (sp, sp), consider the three-loop graph of  $f_L$ , where the lines represent the free propagator

$$G_{\wp}^{(L)}(\boldsymbol{x};\boldsymbol{x}') = \int \frac{d^{d-1}p}{(2\pi)^{d-1}} \sum_{\boldsymbol{m}} \frac{\langle z|m\rangle\langle m|z'\rangle}{p^2 + k_m^2 + \mathring{r}} e^{i\boldsymbol{p}\cdot(\boldsymbol{r}-\boldsymbol{r}')}$$
(4)

between the points x=(r,z) and x'=(r',z'). Here  $\langle z|m\rangle$  and  $k_m^2$  are the orthonormal eigenfunctions and eigenvalues for the BC  $\wp$ , respectively. For example, for  $\wp=$  per one has  $\langle z|m\rangle=L^{-1/2}\,e^{ik_mz}$  with  $k_m=2\pi m/L$  and  $m\in\mathbb{Z}$ , whereas  $\langle z|m\rangle=\sqrt{(2-\delta_{m,0})/L}\,\cos(k_mz)$  for  $\wp=(\mathrm{sp},\mathrm{sp})$ , with  $k_m=\pi m/L$ ,  $m=0,1,\ldots,\infty$ .

The central part of this three-loop graph is the subgraph igoplus, which behaves in the bulk case  $L=\infty$  (for zero external momenta) as  $\mathring{\tau}^{-\epsilon/2}$ , and hence is *infrared singular* at  $T_{c,\infty}$  [27]. However, each of the two other bubbles contributes a factor  $G^{(\infty)}(\boldsymbol{x};\boldsymbol{x})\sim\mathring{\tau}^{1-\epsilon/2}$ . Hence, the limit  $\mathring{\tau}\to 0$  of the overall contribution vanishes [27]. When  $L<\infty$ , each of the two tadpoles  $G_\wp^{(L)}(\boldsymbol{x};\boldsymbol{x})$  for  $\wp=\operatorname{per}$ ,  $(\operatorname{sp},\operatorname{sp})$  can be decomposed into a contribution  $(P_0G_\wp^{(L)}P_0)(\boldsymbol{x};\boldsymbol{x})\sim\mathring{\tau}^{(1-\epsilon)/2}$  from the  $k_m=0$  mode and a remainder  $(Q_0G_\wp^{(L)}Q_0)(\boldsymbol{x};\boldsymbol{x})$ , where  $P_0=\mathbb{1}-Q_0=|0\rangle\langle 0|$ . At  $\mathring{\tau}=0$  we are left with the contributions from the remainder, namely

$$(Q_0 G_{\text{per}}^{(L)} Q_0)(\mathbf{x}; \mathbf{x})|_{\mathring{\tau}=0} = \frac{\Gamma(1 - \epsilon/2)}{2\pi^{2 - \epsilon/2}} \frac{\zeta(2 - \epsilon)}{L^{2 - \epsilon}}$$
 (5)

and

$$(Q_0 G_{\text{sp,sp}}^{(L)} Q_0)(\boldsymbol{x}; \boldsymbol{x})|_{\mathring{\tau}=0} = \frac{\Gamma(1 - \epsilon/2)}{2^{4 - \epsilon} \pi^{2 - \epsilon/2} L^{2 - \epsilon}} \left[ 2\zeta(2 - \epsilon) + \zeta\left(2 - \epsilon, \frac{z}{L}\right) + \zeta\left(2 - \epsilon, \frac{L - z}{L}\right) \right], (6)$$

where  $\zeta(s,a) = \sum_{j=0}^{\infty} (j+a)^{-s}$  is the Hurwitz zeta function.

The zero-mode contribution  $[(P_0G_\wp^{(L)}P_0)(\boldsymbol{x};\boldsymbol{x}')]^2$  of  $\bigcirc$  must be integrated over the parallel separation  $\boldsymbol{r}-\boldsymbol{r}'$ . The result behaves  $\sim \mathring{\tau}^{-(1+\epsilon)/2}$ . Combined with the  $(Q_0G_\wp^{(L)}Q_0)$  parts of the tadpoles,

4 EUROPHYSICS LETTERS

it produces a contribution that diverges as  $\mathring{\tau} \to 0$ . Thus the loop expansion is ill-defined at  $\mathring{\tau} = 0$  for these two BC  $\wp = \mathrm{per}$  and  $(\mathrm{sp}, \mathrm{sp})$ . Evidently, this breakdown should occur more generally whenever a  $k_m = 0$  mode is present, which is not the case for  $\wp = \mathrm{ap}$ , (D, D), and  $(D, \mathrm{sp})$ .

The origin of this breakdown is a deficiency of Landau theory: Whenever the free propagator involves a  $k_m=0$  mode, it predicts a transition for the bulk and the film of finite thickness L at the same critical value  $\mathring{\tau}=0$ . The remedy is a reorganization of the perturbation series. The  $k_m=0$  mode must be split off and treated in the background of the  $k\neq 0$  modes. As a result of its coupling to the latter, the zero mode becomes massive at  $T_{c,\infty}$  for  $L<\infty$ .

To formulate such an expansion, we decompose  $\phi$  as  $\phi(\boldsymbol{x}) = \varphi(\boldsymbol{r}) + \psi(\boldsymbol{x})$  into its k=0 mode contribution  $\varphi(\boldsymbol{r})$  and its orthogonal component  $\psi$  with  $\int_0^L dz \, \psi(\boldsymbol{r},z) = 0$ . Integrating out  $\psi$  defines us an effective d-1 dimensional field theory with the Hamiltonian

$$\mathcal{H}_{\text{eff}}[\varphi] = -\ln \text{Tr}_{\psi} e^{-\mathcal{H}[\varphi + \psi]}. \tag{7}$$

Let us introduce the free-energy part  $F_{\psi}$  and the average  $\langle ... \rangle_{\psi}$  by

$$F_{\psi} \equiv -\ln \operatorname{Tr}_{\psi} e^{-\mathcal{H}[\psi]} , \qquad \langle \ldots \rangle_{\psi} \equiv e^{F_{\psi}} \operatorname{Tr}_{\psi} \left( \ldots e^{-\mathcal{H}[\psi]} \right). \tag{8}$$

Then we have

$$\mathcal{H}_{\text{eff}}[\varphi] = F_{\psi} + \mathcal{H}[\varphi] - \ln\langle e^{-\mathcal{H}_{\text{int}}[\varphi,\psi]} \rangle_{\psi}$$
(9)

with

$$\mathcal{H}_{\text{int}}[\varphi,\psi] \equiv \int_{0}^{L} dz \int_{\mathbb{R}^{d-1}} d^{d-1}r \left[ \frac{\mathring{u}}{4} \varphi^{2} \psi^{2} + \frac{\mathring{u}}{6} (\varphi \cdot \psi) \psi^{2} \right]$$
 (10)

and

$$\mathcal{H}[\varphi] = \int_{\mathbb{R}^{d-1}} d^{d-1}r \left[ \frac{L}{2} (\partial_{r} \varphi)^{2} + \frac{\mathring{r}L}{2} \varphi^{2} + \frac{\mathring{u}L}{4!} \varphi^{4} \right]. \tag{11}$$

The last term in Eq. (9) gives loop corrections  $\sum_{l=1}^{\infty} \mathcal{H}_{\text{eff}}^{[l]}[\varphi]$ . For the one-loop contribution, one obtains

$$\mathcal{H}_{\text{eff}}^{[1]}[\varphi] = \frac{1}{2} \operatorname{Tr} \ln \left[ \mathbb{1} + (\mathring{u}/6) G_{\psi}^{(L)} \left( \delta_{\alpha\beta} \varphi^2 + 2\varphi_{\alpha} \varphi_{\beta} \right) \right]$$

$$= -\varphi \varphi \varphi \varphi - \varphi \varphi \varphi \varphi + \dots, \qquad (12)$$

where the dashed lines represent free  $\psi$ -propagators  $G_{\psi}^{(L)}=Q_0G_{\wp}^{(L)}Q_0$ , while the gray bars indicate  $\varphi$  legs.

Added to  $\mathcal{H}[\varphi]$ , the first graph in Eq. (12) produces the shift

$$\mathring{\tau} \to \mathring{\tau}_{\wp}^{(L)} \equiv \mathring{\tau} + \delta \mathring{\tau}_{\wp}^{(L)} \quad \text{with} \quad \delta \mathring{\tau}_{\wp}^{(L)} = \frac{\mathring{u}}{2} \frac{n+2}{3} \int_{0}^{L} \frac{dz}{L} \left( Q_0 G_{\wp}^{(L)} Q_0 \right) (\boldsymbol{x}; \boldsymbol{x}) , \tag{13}$$

so that the free  $\varphi$ -propagator  $G_{\varphi}^{(L)}$  acquires an L-dependent mass at  $\mathring{\tau}=0$ . The second graph in Eq. (12) yields a nonlocal  $\varphi^2\varphi^2$  interaction; the suppressed ones correspond to similar nonlocal interactions involving more than two  $\varphi^2$  operators. The two-loop term  $\mathcal{H}_{\mathrm{eff}}^{[2]}[\varphi]$  involves two contributions  $\varphi\varphi$ ; a local one giving an  $O(\mathring{u}^2)$  correction to the shift  $\delta\mathring{\tau}_{\wp}^{(L)}$ , and a nonlocal one whose interaction potential is proportional to  $\int_0^L dz \int_0^L dz' \, [G_{\psi}(\boldsymbol{x}, \boldsymbol{x}')]^3$ .

Upon substituting the results (5) and (6) into Eq. (13), the shifts  $\delta \mathring{\tau}_{per}^{(L)}$  and  $\delta \mathring{\tau}_{sp,sp}^{(L)}$  can be computed in a straightforward manner. At  $\mathring{\tau}=0$ , one obtains

$$\delta \mathring{\tau}_{\text{per}}^{(L)} = 2^{2-\epsilon} \, \delta \mathring{\tau}_{\text{sp,sp}}^{(L)} = \mathring{u} \, \frac{n+2}{6} \, \frac{\Gamma(1-\epsilon/2) \, \zeta(2-\epsilon)}{2\pi^{2-\epsilon/2} \, L^{2-\epsilon}}. \tag{14}$$

We can now set up a Feynman graph expansion, utilizing  $\hat{G}_{\varphi}(\boldsymbol{p}) = \left[L\left(p^2 + \mathring{\tau}_{\wp}^{(L)}\right)\right]^{-1}$  as free propagator in the d-1 dimensional momentum space and employing dimensional regularization. Since  $\hat{G}_{\varphi}(\boldsymbol{p})$  remains massive at  $\mathring{\tau} = 0$  when  $L < \infty$ , the Feynman graphs are infrared finite as long as  $\mathring{\tau} \geq 0$ . Owing to our reorganization of perturbation theory, the breakdown encountered in the conventional expansion in terms of  $G_{\wp}^{(L)}$  is avoided. Note also that the correct bulk expressions are recovered as  $L \to \infty$  since the contributions from the zero mode vanish. For example, the term  $F_{\psi}$  in Eq. (9) yields the bulk free energy when  $L \to \infty$ . Indeed, setting  $T = T_{c,\infty}$  and denoting the analog of  $f_{\wp}^{\mathrm{res}}$  for  $F_{\psi}$  as  $f_{\psi;\wp}^{\mathrm{res}}$  we find

$$\frac{L^{d-1}}{n} f_{\psi,\wp}^{\text{res}} \Big|_{T_{c,\infty}} = a_{\wp}^{(0)}(\epsilon) + \frac{n+2}{4!} a_{\wp}^{(1)}(\epsilon) \, \mathring{u} L^{\epsilon} + O(\mathring{u}^2 L^{2\epsilon})$$
(15)

with

$$a_{\text{per}}^{(0)}(\epsilon) = 2^{4-\epsilon} a_{\text{sp,sp}}^{(0)}(\epsilon) = -\frac{\Gamma(2-\epsilon/2)}{\pi^{2-\epsilon/2}} \zeta(4-\epsilon) ,$$

$$a_{\text{per}}^{(1)}(\epsilon) = 2^{-2} \pi^{\epsilon-4} \Gamma^{2} (1-\epsilon/2) \zeta^{2} (2-\epsilon) ,$$

$$a_{\text{sp,sp}}^{(1)}(\epsilon) = \frac{\pi^{1-\epsilon}}{4^{3-\epsilon}} \frac{2 \zeta^{2} (\epsilon-1) + \zeta(2\epsilon-2)}{2 \cos^{2} (\pi \epsilon/2) \Gamma^{2} [(3-\epsilon)/2]} .$$
(16)

KD's two-loop results for  $f_\wp|_{T_{c,\infty}}$  with  $\wp=\mathrm{per}$ ,  $(\mathrm{sp},\mathrm{sp})$  follow from Eqs. (15) and (16), as they should because the zero-mode contributions to  $f_\wp^{\mathrm{res}}$  of order  $\mathring{u}^0$  and  $\mathring{u}$  vanish at  $T_{c,\infty}$ . However, the  $\wp$ -dependent part of  $\mathcal{H}_{\mathrm{eff}}[\wp]$  gives additional contributions. The leading ones correspond to one- and two-loop terms of a  $\wp^4$  theory in d-1 dimensions with mass coefficient  $\mathring{\tau}_\wp^{(L)}$  and coupling constant  $\mathring{u}/L$ , as the rescaling  $L^{1/2}\wp \to \wp$  in Eq. (11) shows. At  $T_{c,\infty}$ , they yield L-dependent contributions to  $f_\wp^{\mathrm{res}}$  proportional to  $(\delta\mathring{\tau}_\wp^{(L)})^{(3-\epsilon)/2} \sim L^{1-d}(\mathring{u}L^\epsilon)^{(3-\epsilon)/2}$  and  $(\mathring{u}/L)(\delta\mathring{\tau}_\wp^{(L)})^{1-\epsilon} \sim L^{1-d}(\mathring{u}L^\epsilon)^{2-\epsilon}$ , respectively. Including only the first one, we arrive at

$$\frac{L^{d-1}}{n} \left[ f_{\wp}^{\text{res}} - f_{\psi;\wp}^{\text{res}} \right]_{T_{c,\infty}} = A_{\wp}(\epsilon) \left( \frac{n+2}{4!} \mathring{u} L^{\epsilon} \right)^{(3-\epsilon)/2} + \dots$$
 (17)

with

$$A_{\rm per}(\epsilon) = 2^{(2-\epsilon)(3-\epsilon)/2} A_{\rm sp,sp}(\epsilon) = -\frac{\Gamma[(\epsilon-3)/2]}{2^{4-\epsilon}} \left[ \frac{2\Gamma(1-\epsilon/2)\zeta(2-\epsilon)}{\pi^{(6-\epsilon)/2}} \right]^{(3-\epsilon)/2}.$$
(18)

To combine these results with RG-improved perturbation theory, we follow KD. We utilize the reparametrizations ( $\mathring{u}=2^d\pi^{d/2}Z_u\mu^\epsilon u,\,\mathring{\tau}=\mu^2Z_\tau\tau,\ldots$ ) of bulk and surface quantities of the corresponding semi-infinite theories [22], and fix the additional additive (bulk and surface) counterterms  $f_L$  requires such that  $f_{L,\mathrm{ren}}$ , its renormalized counterpart, vanishes at  $\tau=1$  together with its 1st and 2nd  $\tau$ -derivatives [28]. To obtain the critical Casimir amplitudes  $\Delta_\wp$ , we must express  $f_\wp^{\mathrm{res}}$  in terms of renormalized variables, set  $\mu L=1$  and  $\tau=0$ , and evaluate it at the fixed-point value  $u^*=3\epsilon/(n+8)+O(\epsilon^2)$ . Upon expanding in powers of  $\epsilon$ , we find ( $\gamma=1$ ) Euler-Mascheroni constant)

$$\frac{\Delta_{\text{per}}}{n} = -\frac{\pi^2}{90} + \frac{\pi^2 \epsilon}{180} \left[ 1 - \gamma - \ln \pi + \frac{2\zeta'(4)}{\zeta(4)} + \frac{5}{2} \frac{n+2}{n+8} \right] - \frac{\pi^2}{9\sqrt{6}} \left( \frac{n+2}{n+8} \right)^{3/2} \epsilon^{3/2} + O(\epsilon^2)$$
 (19)

and

$$\frac{\Delta_{\text{sp,sp}}}{n} = -\frac{\pi^2}{1440} + \frac{\pi^2 \epsilon}{2880} \left[ 1 - \gamma - \ln(4\pi) + \frac{5}{2} \frac{n+2}{n+8} + \frac{2\zeta'(4)}{\zeta(4)} \right] - \frac{\pi^2}{72\sqrt{6}} \left( \frac{n+2}{n+8} \right)^{3/2} \epsilon^{3/2} + O(\epsilon^2) .$$
(20)

**6** EUROPHYSICS LETTERS

The  $O(\epsilon^{3/2})$  terms result from the  $O(\mathring{u}^{(3-\epsilon)/2})$  contributions in Eq. (17). Obviously, the latter also implies contributions of the form  $\epsilon^{k+3/2} \ln^k \epsilon$  with  $k \in \mathbb{N}$ . Furthermore, the terms  $(\mathring{u}/L)(\delta\mathring{\tau}_\wp^{(L)})^{1-\epsilon} \sim \mathring{u}^{2-\epsilon}$  mentioned above yield contributions of the form  $\epsilon^{k+2} \ln^k \epsilon$ .

Can the appearance of the  $\epsilon^{3/2}$  and unconventional higher-order terms be checked by alternative means? This is indeed possible: The limiting value  $\lim_{n\to\infty} \Delta_{\mathrm{per}}/n$  can be obtained from the exact solution of the mean-spherical model (expressed in terms of the function  $Y_0$  of [29], it becomes  $Y_0(0,0)$ ). Solving the corresponding self-consistent equations iteratively with  $\epsilon>0$  reproduces the  $n\to\infty$  limit of all terms on the right-hand side of Eq. (19) and shows the existence of higher-order contributions of the mentioned form [30].

In Table I we give the values of  $\Delta_{\wp}$  Eqs. (19) and (20) predict for  $n=1,2,3,\infty$  upon setting  $\epsilon=1$ .

Table I – Estimated values of  $\Delta_{\wp}(d,n)/n$  for d=3. Following [9], we have included the d=3 values of  $\Delta_{\mathrm{sp,sp}}$ , although they are probably of little physical interest because the special surface transition is not expected to occur at d=3 in the  $O(n\geq 2)$  case, unless surface couplings of infinite strengths are allowed.

n	1	2	3	$\infty$
$\Delta_{\rm per}(3,n)/n$	$-0.1967^{a}$	$-0.2147^{a}$	$-0.2311^a$	$-0.4668^a$
	$-0.1105^{b}$	$-0.1014^{b}$	$-0.0939^{b}$	$-0.0192^{b}$
	$-0.1526^{c}$			$-0.1531^d$
$\Delta_{\rm sp,sp}(3,n)/n$	$-0.0224^{a}$	$-0.0252^{a}$	$-0.0278^{a}$	$-0.0619^a$
	$-0.0117^{b}$	$-0.0111^{b}$	$-0.0106^{b}$	$-0.0059^{b}$

<sup>&</sup>lt;sup>a</sup> Values obtained by setting  $\epsilon = 1$  in Eqs. (19) and (20).

For comparison, the corresponding  $O(\epsilon)$  estimates are also listed, along with a MC estimate [31] and an exact  $n=\infty$  result [29, 32]. A known problem of the  $O(\epsilon)$  results for  $\Delta_{\rm per}$  is the seemingly incorrect n-dependence of the predicted d=3 values, whose deviations from the exact  $n=\infty$  value increase monotonically as n grows (see Fig. 12.8 of [12] and [16]), although the MC estimate for n=1 is very close to the exact  $n=\infty$  value. The  $\epsilon^{3/2}$  term modifies the n dependence, yielding an estimate for  $-\Delta_{\rm per}/n$  that increases with n.

In summary, we have shown the following: (i) the  $\epsilon$  expansions of quantities such as Casimir amplitudes are ill-defined at  $T_{c,\infty}$  when the BC gives a zero mode in Landau theory. (ii) The reformulation of field theory presented here yields well-defined small- $\epsilon$  expansions for temperatures  $T \geq T_{c,\infty}$ . In the cases of  $\Delta_{\rm per}$  and  $\Delta_{\rm sp,sp}$ , these expansions involve fractional powers and logarithms of  $\epsilon$ . Clearly, more work is necessary to explore the potential of such expansions for reliable extrapolations to d=3.

In typical experimental situations one expects to have either Robin BC  $\partial_n \phi = \mathring{c}_j \phi$  (which in the long-scale limit normally should map on (D,D) BC) or symmetry-breaking  $(+,\pm)$  BC (classical liquids). However, experimental situations corresponding to near-critical enhancement of surface interactions on both plates are conceivable. In that case a crossover from an initial behavior characteristic of  $(\mathrm{sp},\mathrm{sp})$  BC should occur. Clearly, proper treatments of this crossover must take into account the findings described above. Needless to say, that in MC simulations periodic BC are *the* preferred choice, and that simulations dealing with  $(\mathrm{sp},\mathrm{sp})$  BC were performed as well [33].

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 $<sup>^{</sup>b}$   $O(\epsilon)$  results [9], evaluated at  $\epsilon=1$ .

<sup>&</sup>lt;sup>c</sup> MC results according to [31].

<sup>&</sup>lt;sup>d</sup> Exact value  $-2\zeta(3)/(5\pi)$  according to [32] and [29].

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